International Journal of Mass Spectrometry 315 (2012) iii–v

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

journal homepage: www.elsevier.com/locate/ijms

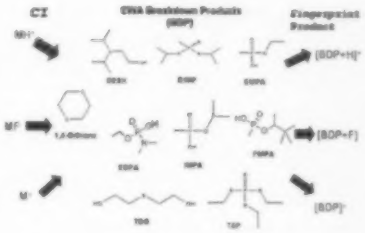
Contents

1–7

Survey of ion energetics properties of chemical weapon agent (CWA) breakdown products using G3(MP2) theory

Anthony J. Midey, Thomas M. Miller, A.A. Viggiano

► We calculated the ion energetics of chemical weapon agent breakdown products. ► Positive ion reac-tions should best ionize these products for spectrometry methods. ► G3(MP2) data show proton or charge transfer reactions create signature products.

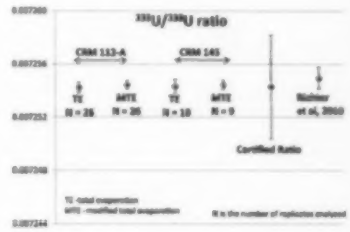


8–14

Uranium isotope abundance ratios in natural uranium metal certified reference material 112-A

K. Mathew, P. Mason, A. Voeks, U. Narayanan

► The $^{234}U/^{238}U$ and $^{235}U/^{238}U$ isotope-amount ratios in natural uranium metal certified reference material 112-A and CRM 145 are char-acterized. ► The $^{235}U/^{238}U$ ratios from two analytical techniques (total evaporation and modified total evaporation) are in agreement. ► Uncertainties in the CRM 112-A $^{235}U/^{238}U$ and $^{234}U/^{238}U$ ratios are calculated following the GUM. ► The certified isotope abundance ratios are in excellent agreement with the values obtained in the IRMM measurement campaign. ► Traceability of the measured isotopic ratios with SI units and with US nuclear reference materials is established through the use of CRM U030-A.

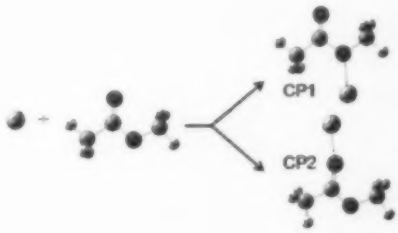


15–21

Intracluster ion–molecule reactions between V^+ and methyl acetate or ethyl acetate clusters

Dababrata Paul, Kiryong Hong, Tae Kyu Kim, Jun-Sik Oh, Kwang-Woo Jung

► Intracluster ion–molecule reactions of vanadium ion and alkyl acetate were studied. ► Competitive V^+ insertions and fragmentation mechanism were proposed. ► Evidence for H atom migration within heteroclusters is provided by isotope-labeling experiments. ► Density functional theory calculations rationalize the reaction pathways and energetics.



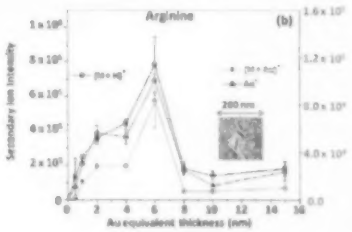
Elsevier B.V.
http://dx.doi.org/10.1016/S1387-3806(12)00139-X

22–30

Metal condensates for low-molecular-weight matrix-free laser desorption/ionization

A. Prabhakaran, J. Yin, B. Nysten, H. Degand, P. Morsomme, T. Mouhib, S. Yunus, P. Bertrand, A. Delcorte

▶ This article demonstrates the interest of metal nanoislands condensed on top of organic surfaces by PVD to enhance the characteristic ion yields of the underlying materials upon UV laser ablation. ▶ The characteristic ion yield enhancements are up to 4 orders of magnitude with respect to pristine samples. ▶ It is a solvent-free and matrix-free approach to laser ablation. ▶ The observed signal enhancement is explained by increased laser absorbance (ablation) and work function (ionization). ▶ The main potential of the method concerns the imaging of organic samples using laser ablation.

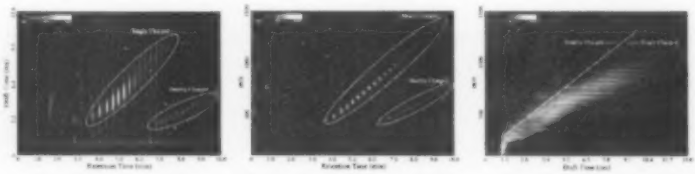


31–39

Comprehensive two-dimensional separation for the analysis of alkylphenol ethoxylates employing hydrophilic interaction chromatography coupled with ion mobility-mass spectrometry

Qiang Ma, Guang-Cheng Xi, Chao Wang, Hua Bai, Qing Zhang, Hai-Wei Xi, Zi-Ming Wang, Liang-Hong Guo

▶ A novel two-dimensional system combing HILLIC and IM-MS was constructed for the separation and analysis of APEOs. ▶ The developed plane exhibited unique selectivity and increased peak capacity. ▶ Ion mobility approach demonstrated attractive potential to remove isobaric interference.

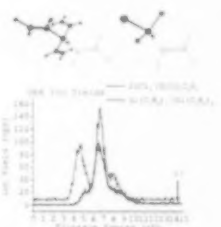


40–45

Dissociative electron attachment to the silane derivatives trichlorovinylsilane ($SiCl_3C_2H_3$), tetravinylsilane ($Si(C_2H_3)_4$) and trimethylvinylsilane ($Si(CH_3)_3C_2H_3$)

Jaroslav Kočišek, Eugen Illenberger, Štefan Matejčík

▶ DEA to selected vinylsilanes is studied in 0eV-12 eV electron energy range. ▶ Resonant structures in particular reaction channels are revealed. ▶ The influence of different functional groups is illuminated. ▶ Conclusions about the role of silicon bonding are given.

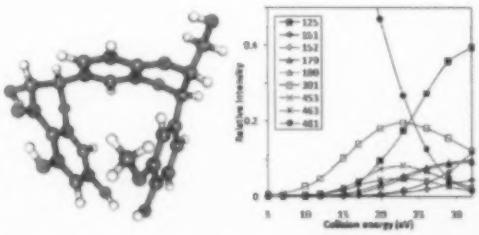


46–54

Collision induced dissociation study of the major components of silymarin

Ákos Kuki, Bernadett Biri, Lajos Nagy, György Deák, József Kalmár, Attila Mándi, Miklós Nagy, Miklós Zsuga, Sándor Kéki

▶ Energy dependence of the fragmentation of the silymarin components is reported. ▶ Survival yield and breakdown curve plots are presented. ▶ Distinct fragmentation behavior of silybins and isosilybins was observed. ▶ In the basis of MS/MS experiments and conformational analysis the observations were explained.

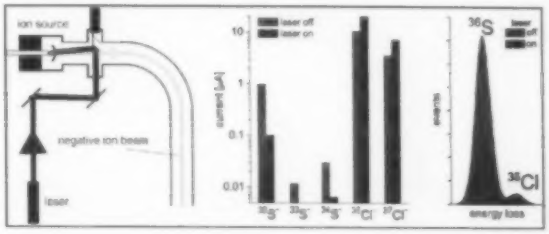


55–59

Light induced suppression of sulfur in a cesium sputter ion source

Martin Martschini, Johan Rohlén, Pontus Andersson, Robin Golser, Dag Hanstorp, Anton O. Lindahl, Alfred Priller, Peter Steier, Oliver Forstner

► The effect of cw laser light on the production of S^- and Cl^- was studied. ► The S^- current was reduced by one order of magnitude with 100 mW of laser power. ► The Cl^- current became enhanced. ► Time structure and power dependence of the effect were investigated. ► The effect was successfully applied in a regular AMS 36Cl measurement.

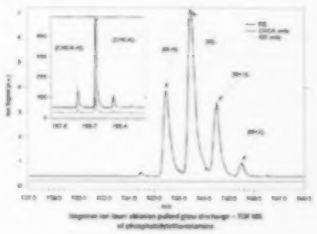


60–65

Negative ion laser ablation glow discharge-time of flight mass spectrometry of organic molecules

G. Lotito, D. Günther

► Negative ion (NI) measurements of some organic compounds. ► Measurements first done by laser ablation coupled to pulsed glow discharge TOF-MS. ► Measurements then performed by MALDI TOF-MS. ► NI measurements provide complementary info to positive ion mode in both techniques. ► Ionization in NI mode of this new technique less matrix dependent than in MALDI.

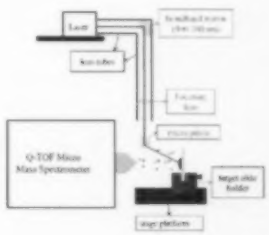


66–73

Atmospheric pressure visible-wavelength MALDI-MS

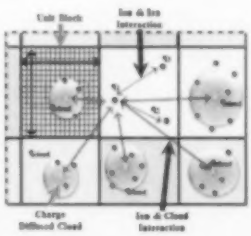
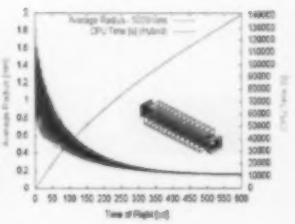
Zhen Sun, Eric W. Findsen, Dragan Isailovic

► An atmospheric pressure (AP) visible-wavelength MALDI source was coupled to a Q-TOF MS. ► Visible-wavelength AP MALDI-MS and MS/MS analyses of a variety of samples are reported for the first time. ► Several visible-wavelength absorbing dyes were successfully studied and utilized as MALDI matrices. ► Three dyes were reported as novel visible-wavelength MALDI matrices.



74–80

A hybrid approach to calculating Coulombic interactions: An effective and efficient method for optimization of simulations of many ions in quadrupole ion storage device with SIMION

Kenichiro Saito, Peter T.A. Reilly, Eiko Koizumi, Hideya Koizumi

► Developed a new algorithm for calculating time consuming ion–ion repulsive interaction. ► Demon-stration of the accuracy of the algorithm. ► Significant improvement in the computational time.